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Lagrangian Statistical Simulation of Concentration Mean and Fluctuation Fields

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ABSTRACT

Lagrangian statistical (Monte Carlo) simulations of the mean and fluctuating concentration fields due to turbulent dispersion are critically reviewed. Attention has been restricted to work in which particle trajectories are modeled directly, which in effect means simulations based on the Langevin equation (or in finite difference form, Markov-chains) and its generalization. The material covered has been selected and presented so as to achieve an orderly progression from simple to more complex turbulent flows. At present this field involves many heuristic modeling assumptions and an attempt is made to justify some of these by appeal to special and limiting cases.

1. Introduction

The past five years have seen a rapid growth in interest in Lagrangian simulations of turbulent dispersion. The techniques employed can be broadly grouped into two categories. In the first, dispersion and concentration statistics are estimated by tracking marked fluid particles through an Eulerian velocity field obtained either by solving the Navier-Stokes equations with some closure assumption (Deardorff and Peskin, 1970; Peskin, 1974; Kowalski and Peskin, 1981) or by stochastic methods (Kraichnan, 1970; Lindburgh and Thompson, 1974; Drummond *et al.*, 1984). Alternatively particle trajectories can be generated directly using a stochastic model for Lagrangian velocities, an approach initiated by Taylor (1921). Clearly the first approach provides a direct connection between Eulerian and Lagrangian velocity statistics whereas the second requires a knowledge of, or assumptions about, Lagrangian statistics. The latter is generally more efficient and has greater potential for application to practical dispersion problems in the atmosphere but requires careful analysis and testing. In this review, with the notable exception of Lamb's simulations of dispersion for convective turbulence (Lamb, 1982), we restrict attention to dispersion studies involving the direct simulation of particle trajectories. As will become apparent, these are based almost exclusively on the Markov-chain or Langevin equation model for the Lagrangian velocity.

Even within this restricted framework, we have attempted to treat the subject critically, rather than exhaustively, by concentrating on material which emphasizes important features of the underlying physics. In section 2 we outline the Lagrangian approach to estimating concentration statistics and indicate briefly its advantages over the more conventional Eulerian methods. The main body of the review deals separately with estimation of the mean concentration, $\langle c \rangle$, (where $\langle\ \rangle$ denotes the ensemble mean) in section 3 and of the concentration variance, $\langle c'^2 \rangle = \langle c^2 \rangle - \langle c \rangle^2$, in section 4. In both cases the physical basis for existing models is first considered for stationary homogeneous turbulence. Extensions to the models are then developed through a sequence of idealized conditions of increasing complexity (sheared homogeneous turbulence, neutral boundary layer, stability effects, convection) for which comparisons with known results (exact or from other modeling techniques; special limiting cases; field or laboratory data) can be made.

2. Lagrangian versus Eulerian

The Lagrangian treatment of statistics of the concentration field is based on relations involving displacement statistics of "marked particles." For example the ensemble-mean concentration at a "point" z at time t is (Tennekes and Lumley, 1972, p. 236)

$$\langle c(\underline{x}, t) \rangle = \int_{-\infty}^{t} \int_{V} S(\underline{x}', t') P_1(\underline{x}', t'; \underline{x}, t) d\underline{x}' dt', \quad (2.1)$$

and the two-point covariance is (see for example Monin and Yaglom 1971, p. 589, *et seq*)

$$\langle c(\underline{x}_1, t) c(\underline{x}_2, t) \rangle = \int_{-\infty}^{t} \int_{V} S(\underline{x}'_1, t'_1) S(\underline{x}'_2, t'_2) \times P_2(\underline{x}'_1, \underline{x}'_2, t'_1, t'_2; \underline{x}_1, \underline{x}_2, t) d\underline{x}'_1 d\underline{x}'_2 dt'_1 dt'_2. \quad (2.2)$$

Here $S(\underline{x}, t)$ is the source distribution and P_1 and P_2 are one- and two-particle probability density functions. These equations can be interpreted in terms of dispersion of marked particles either forward in time from

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the source location $(\underline{x}', t')$ to the sampling location $(\underline{x}, t)$, or backward in time from the sampling location to the source. For incompressible flow, Lundgren (1981) and Egbert and Baker (1984) show these two interpretations to be equivalent. This is generally the case for the mean concentration field. For the two-particle models discussed in section 4 (which are one-dimensional and hence do not satisfy the incompressibility constraint), Sawford (1983a, 1984a) has shown that the reverse diffusion interpretation is appropriate since it deals with the mass-specific concentration and so corrects for spurious concentration fluctuations introduced by fluctuations in the total fluid density.

Traditional Eulerian methods of modeling turbulent dispersion use a set of moment equations which can be derived by Reynolds-averaging the Eulerian conservation equation for c. As pointed out by Lamb (1980), closure of the latter set of equations involves approximate relations among certain joint moments of the velocity and concentration fields. Such approximations clearly depend on the concentration field itself and so are not uniformly valid. For example, the gradient transfer hypothesis which leads to the diffusion equation requires that the length scale of the turbulence be small compared with that of the contaminant distribution and, as is well known (Pasquill and Smith, 1983, chap. 3), breaks down close to "point" sources but is asymptotically valid for large travel time. It is possible to force Eulerian closures to correctly model the mean concentration field close to an isolated point source either by prescribing an appropriate time-dependent diffusivity (Deardorff, 1978) or by forcing a second-order closure scheme to generate such a diffusivity (Sykes *et al.*, 1984). However, for multiple sources each release must then be treated separately and in general at any point in the fluid different diffusivities are appropriate for material from different plumes. This is clearly illogical, as pointed out by Taylor (1959).

In contrast, the unknown quantities P_1 and P_2 are determined solely by the velocity field. Thus, although the Lagrangian approach in which P_1 and P_2 are calculated by modeling particle trajectories does not avoid the need for approximations (the "closure problem" is unavoidable) any approximations made involve only the velocity field. Calculation of concentration moments through (2.1) and (2.2) is quite a separate process and can be carried out for an arbitrary source distribution. The assumptions made in Lagrangian modeling thus do not depend on the concentration field or the source distribution and in this sense, are uniformly valid.

Lagrangian models are simpler and physically more transparent than higher-order Eulerian closure models. They also possess the computational advantages of being potentially more efficient than Eulerian methods generally (since calculations involve only those portions of the fluid which are marked and therefore of interest) and free from problems such as numerical diffusion. Their main disadvantage is that they cannot be used if the contaminant is involved in nonlinear chemical reactions with other species (Lamb, 1980).

3. Mean concentration field

a. *Stationary homogeneous turbulence*

All recent Lagrangian simulations of turbulent dispersion have been based implicitly on (or can be derived from) the Langevin equation or a generalization of it. The Langevin equation is well known in the theory of Brownian motion and in the present context can be written (Durbin, 1980a,b; 1983).

$$dW(t) = -\frac{W}{t_L}\,dt + \sigma_w\left(\frac{2}{t_L}\right)^{1/2} d\mathcal{W}_t, \qquad (3.1)$$

where $W(t)$ is a component of the Lagrangian velocity, and $d\mathcal{W}_t$ is a Gaussian, white-noise stochastic process with mean zero and variance dt. With the initial condition that $W(0)$ is a Gaussian random variable with mean zero and variance σ_w^2 it is easily shown (Durbin, 1983; Legg and Raupach, 1982) that $W(t)$ is also Gaussian with mean zero and variance σ_w^2 and that the autocorrelation is

$$R_L(\tau) = \langle W(t)W(t+\tau)\rangle/\sigma_w^2 = \exp(-\tau/t_L). \qquad (3.2)$$

The Langevin equation thus models "memory" through the integral time scale t_L. The position of the particle is given by integrating

$$dZ = W dt. \qquad (3.2)$$

There has been no rigorous derivation of the Langevin equation from the Navier Stokes equations and its justification rests on the correspondence between its properties and those observed in homogeneous turbulence. Some of these are summarized in Table 1. Note that the acceleration is modeled as white noise ($d\mathcal{W}_t$ is white noise), whereas in three-dimensional turbulence the acceleration is significantly correlated over lags of order $t_k = \mathrm{Re}^{-1/2}t_L$, the Kolmogorov time scale, where Re is the Reynolds number. Application of the Langevin equation is thus restricted to high-Re three-dimensional turbulence and to time $t \gg t_k$.

In finite difference form the Langevin equation becomes the so-called Markov-chain model used originally by Taylor (1921),

$$W_{n+1} = W_n R_L(\delta t) + \sigma_w[1 - R_L^2(\delta t)]^{1/2} W''_{n+1}, \qquad (3.3)$$

where the subscripts of W refer to the time steps and W''_{n+1} is a Gaussian random variable with zero mean and unit variance. The particle position is given by

$$Z_{n+1} = Z_n + W_n \delta t. \qquad (3.4)$$

In order to properly resolve memory effects δt must be small compared with t_L, typically $\delta t < 0.1 t_L$. In practice then, (3.3) and (3.4) are solved for a suitably

TABLE 1. Langevin properties in stationary homogeneous turbulence.

Property	Langevin form
finite time scale, t_L	$R_L(t) = \exp(-t/t_L)$
correct inertial range	$R_L(t) \sim 1 - t/t_L \; (t \ll t_L)$
acceleration correlated for time $Re^{-1/2}t_L$ in high-Re three-dimensional turbulence	"white-noise" acceleration
velocity distribution	$P(w)$ Gaussian
particle distribution	$P(z)$ Gaussian
mean concentration	$\langle C(z) \rangle$ Gaussian
diffusion equation limit	$\sigma_z^2 = 2\sigma_w^2 t t_L (t \gg t_L)$ $K = \sigma_w^2 t_L$

large number, N_t, of particle trajectories over which appropriate averages can be taken to evaluate statistics such as $\sigma_z^2 = \langle Z^2(t) - Z^2(0) \rangle$ and $\langle c(z, t) \rangle$. Details are given by Durbin (1980a) for an instantaneous source and by Legg (1983) for a continuous source. In general the statistical uncertainty in estimates of σ_z^2 and $\langle c(z, t) \rangle$ is proportional to $N_t^{-1/2}$ so that typical one-dimensional (i.e., continuous line source or instantaneous area source) mean-field calculations using $N_t \sim 5 \times 10^3$ are accurate to a few percent. The other factor affecting computational expense, the number of time steps per realization, depends on the problem in hand. For homogeneous turbulence with $\delta t = 0.1 t_L$ integration to the asymptotic diffusion equation limit requires perhaps 50–100 time steps. Similar computational requirements apply to other mean-field calculations. One-dimensional calculations of this magnitude are quite practicable but note that the computational effort increases multiplicatively with dimensionality.

The only properties of the turbulence required as input to the model are σ_w and t_L. Their specification is of more general interest and in a sense independent of the details of the Langevin model. In stationary homogeneous turbulence, Lagrangian and Eulerian single-point velocity moments are equivalent (Lumley, 1962) (i.e. $\langle W^2 \rangle = \sigma_w^2 = \sigma_{wE}^2$, the Eulerian velocity variance) while the Lagrangian time scale is usually assumed proportional to the Eulerian length scale L, of the turbulence,

$$\sigma_w t_L / L = \beta, \tag{3.5}$$

with $\beta \sim 0.35$–0.8 (Pasquill and Smith, 1983, p. 84).

The generalizations which follow are couched in terms of the Langevin equation (3.1) but it should be remembered that calculations proceed through finite difference forms corresponding to (3.3).

b. Neutral boundary layer

This is the simplest inhomogeneous case. In the constant stress region the essential property of the turbulence is that length (and time) scales increase linearly with height above the boundary and the velocity scale is constant. The Langevin equation has been adapted to this situation (Hall, 1975; Reid, 1979; Durbin, 1980b; Durbin and Hunt, 1980; Wilson *et al.*, 1981a; Ley, 1982; Legg, 1983; Davis, 1983) simply by keeping σ_w constant,

$$\sigma_w = b_1 u_*, \tag{3.6}$$

where u_* is the friction velocity, and regarding t_L as a *local* property of the turbulence and hence as a linear function of the particle-position,

$$t_L = b_2 Z(t)/\sigma_w. \tag{3.7}$$

This extended Langevin model satisfies surface layer similarity. For an instantaneous ground-level source (or for $t \gg z_s/u_*$ for a source at height z_s) the center of mass and the vertical dispersion of the particles grow linearly with time,

$$\langle Z(t) \rangle = c_1 u_* t, \tag{3.8a}$$

$$\langle Z^2(t) \rangle = c_2^2 u_*^2 t^2, \tag{3.8b}$$

where c_1 and c_2 are universal constants.

Equations (3.8) show that although the Eulerian mean vertical velocity has been taken to be zero everywhere, the Lagrangian mean velocity, $\langle W(t) \rangle = d\langle Z(t) \rangle / dt = c_1 u_*$, is non-zero; there is a constant mean drift of particles up the gradient in t_L. In physical terms, the source of this mean velocity is that particles moving in the direction of increasing t_L (i.e., upwards) maintain their direction of motion longer on average than particles moving in the direction of decreasing t_L (downward).

It will become apparent that in general σ_w^2 no longer corresponds to the Lagrangian velocity variance. Furthermore, in inhomogeneous turbulence, t_L cannot be regarded as an integral length scale but is better considered to be the local decorrelation time scale,

$$\left| \frac{1}{R_L(\tau)} \frac{dR_L(\tau)}{d\tau} \right|^{-1}_{\tau/t_L \to 0},$$

(Durbin, 1983).

Most authors take σ_w^2 equal to the Eulerian velocity variance σ_{wE}^2, giving (Pasquill and Smith, 1983, p. 72)

$$\sigma_w \approx 1.3 u_*. \tag{3.9}$$

This can be justified by the requirement that the Langevin equation satisfy the small time limit for dispersion from an elevated source, which is just the homogeneous turbulence result (Durbin and Hunt, 1980),

$$\langle Z^2 \rangle - z_s^2 = \sigma_w^2 t^2 = \sigma_{wE}^2(z_s) t^2, \quad (u_* t \ll z_s). \tag{3.10}$$

Although a value of b_2 can be inferred from (3.5) together with Eulerian length-scale data (Hunt and Weber, 1979) this is not very precise. An alternative is to estimate b_2 by requiring that the Langevin equation

match the diffusion equation solution for $u_*t \gg z_s$. The diffusivity is

$$K(z) = \sigma_w^2 t_L = b_1 b_2 u_* z, \tag{3.11}$$

which with (3.9) and the additional assumption of Reynold's analogy for the diffusion of matter and momentum,

$$b_1 b_2 = k, \tag{3.12}$$

where $k \sim 0.4$ is von Karman's constant, fixes b_2.

Asymptotic matching to the diffusion equation can be partly but not conclusively justified by the comparisons with laboratory and field data which are summarized in Table 2. Hall (1975), Legg (1983), Ley (1983) and Davis (1983) modeled dispersion due to the streamwise component of the turbulence as well as the vertical component, concluding that the former effect was small (~5%). Davis (1983) and Durbin and Hunt (1980) also modeled the departure from the surface layer forms (3.6) and (3.7) at greater heights in the boundary layer. This effect should also be relatively unimportant for small distances downwind (such that the bulk of the plume is confined to the bottom half of the boundary layer) and in the atmosphere will be in any case stability dependent. Durbin and Hunt (1980), Wilson *et al.* (1981a), Legg (1983) and Davis (1983) also considered dispersion from elevated sources.

The calculations summarized in Table 2 are all claimed to fit the corresponding data. Here we are mainly interested in the product $b_1 b_2 = K/u_* z$, for which a value of about 0.4 is consistent with diffusion equation matching and the Reynolds analogy. Comparisons against laboratory data (Durbin and Hunt, 1980; Legg, 1983) thus support this matching but comparisons with field data are less clear. The results of Ley (1983) are consistent with the laboratory data, but those of Reid (1979), Wilson *et al.* (1981a) and Davis (1983) suggest the larger value, $b_1 b_2 \sim 0.63$, better fits the data. However, this larger value is inconsistent with the diffusion equation analysis of Nieuwstadt and van Ulden (1978). Since boundary layer properties enter the steady equation for vertical diffusion only through the term $\bar{U}^{-1}(z)\partial/\partial z[K(z)\partial\langle c\rangle/\partial z]$, the solution is determined by the product $kK/u_* z$. Nieuwstadt and van Ulden obtained a good fit to Project Prairie Grass (PPG) and Porton data using $k = 0.35$ and $K/u_* z = 0.47$. These values give the same product (and hence the same diffusion equation solution) as the values $K/u_* z = k = 0.41$ used by Ley (1983). Thus Ley's Langevin simulations of field data are consistent with the diffusion equation analysis of Nieuwstadt and van Ulden, but those of Reid (1979), Wilson *et al.* (1981a) and Davis (1983) (using $k = 0.4$ and $K/u_* z = 0.65$) are not. The reasons for this inconsistency in modeling the field data remain unclear.

An alternative approach is to directly compare diffusion equation predictions with those of the Langevin equation (Legg, 1983; Ley, 1983; Sawford, 1984b). Sawford used (3.11) for σ_w and treated $b_2 = \partial\sigma_w t_L/\partial z$ as a free parameter representing the strength of the inhomogeneity of the turbulence. Then, for a ground-level instantaneous plane source the diffusion equation predictions are (Chatwin, 1968)

$$\langle W(t)\rangle = \partial K/\partial z = b_1 b_2 u_*; \tag{3.13a}$$

$$\langle Z^2(t)\rangle/\langle Z(t)\rangle^2 = 2; \tag{3.13b}$$

$$\langle c(z, t)\rangle = \frac{Q}{\langle Z(t)\rangle} \exp[-z/\langle Z(t)\rangle], \tag{3.13c}$$

where Q is the source strength.

Sawford's calculations show that these diffusion equation results match the Langevin solution only in the limit $b_2 \to 0$, i.e., in the weakly inhomogeneous limit. Physically this corresponds to the well-known condition that the length scale of the turbulence be small compared with that of the cloud of material i.e., $\langle \sigma_w t_L \rangle \ll \langle z \rangle$. For $b_2 \sim 0.3$ (the value obtained by assuming diffusion equation matching and the Reynolds analogy with $k = 0.4$) the diffusion equation differs from the Langevin solution by only a few percent, i.e. there is only a slight inconsistency involved in the matching procedure and the diffusion equation is a good approximation for the asymptotic stage of vertical dispersion in a neutral boundary layer. Raupach's (1983) Langevin simulation using $b_2 = 0.33$ also matches the large-time diffusion limit to within a statistical uncertainty of about 10%.

For strongly inhomogeneous turbulence, $b_2 = \partial\sigma_w t_L/\partial z \not\ll 1$, the diffusion equation is inapplicable and the results (3.13) differ more significantly, even qualitatively, from the Langevin results. Physically, this is because the eddies responsible for dispersion are always larger than the plume. A particularly interesting feature

TABLE 2. Summary of comparison of Langevin simulations for a neutral boundary layer against experiment and theory.

Source	b_1	b_2	$b_1 b_2$	Data	Theory
Hall (1975)	1.3				
Reid (1979)	1.26	0.5	0.64	Porton	similarity
Durbin and Hunt (1980)	1.0	0.4	0.4	Wind tunnel	diffusion
Wilson *et al.* (1981c)	1.25	0.5	0.63	PPG/Elora	diffusion
Ley (1982)	1.3	0.3	0.4	PPG/Porton	diffusion/similarity
Legg (1983)	1.26	0.3	0.38	Wind tunnel	diffusion
Davis (1983)	1.3	0.5	0.65	PPG/Agesta	

of the Langevin solution in this case is evident in Fig. 1(a), which shows that for $b_2 = 2$ concentration profiles for an elevated source evolve to a similarity solution in which the maximum concentration is not at the surface but above it. This point is emphasized in Fig. 1(b) showing the evolution of the height of maximum concentration. This "lift-off" phenomenon reflects the departure from the balance between mean-drift and dispersion described by (3.13b), which in the diffusion equation solution ensures that the concentration maximum is at the surface. Since the flux of material is upwards, the region of positive mean-concentration gradient below the maximum is a region of countergradient flux. We return to this phenomenon and give an example of its occurrence in the atmosphere in section 3d.

Despite the inconsistencies in the comparisons with field data, it appears that the diffusion equation is a reasonable approximation to the Langevin solution in a neutral boundary layer for $u_*t/z_s \gg 1$ and that therefore the value $b_2 = 0.3$ derived by the matching procedure is appropriate. However, computations show that the diffusion equation concentration profile (3.13c) is a good approximation only after $t \sim 20t_L(z_s)$ [see also Fig. 5 of Durbin and Hunt (1980)]. The capability of treating the initial stage of dispersion from an elevated source and the transition to the similarity limit at these large times is the main practical advantage the Langevin simulation has over the diffusion equation.

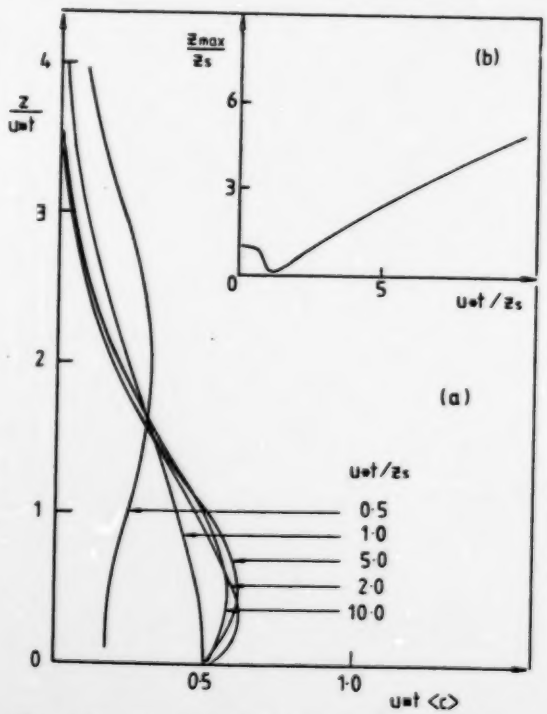

FIG. 1. Langevin simulations for a strongly inhomogeneous boundary layer showing (a) concentration profiles at various times; (b) the height of maximum concentration as a function of time.

c. *Spatially varying velocity scale*

For turbulence where σ_w varies with height, for example in crop canopies (Legg and Raupach (1982); Raupach and Thom, 1981; Wilson *et al.*, 1982) or in non-neutral boundary layers (Kaimal *et al.*, 1976), extension of the Langevin equation is less straightforward. In the weakly inhomogeneous limit the diffusion equation should apply with a mean drift of particles up the gradient of diffusivity, i.e.

$$\langle W \rangle = \frac{d}{dz}(\sigma_w^2 t_L), \quad (\langle W \rangle \to 0).$$

However, numerical experiments (Wilson *et al.*, 1981b; McNider, 1981; Legg and Raupach, 1982) show that merely using the local value of σ_w in the Langevin equation does not generate that component of the drift, $t_L d\sigma_w^2/dz$, due to the gradient in σ_w and that as a consequence particles accumulate in regions of low turbulence kinetic energy. This difficulty can be overcome by adding a drift correction a_d, to the Langevin equation which then becomes in general

$$dW = -\frac{W}{t_L(Z)}\,dt + \sigma_w(Z)\left(\frac{2}{t_L(Z)}\right)^{1/2} d\mathcal{W}_t + a_d dt. \tag{3.14}$$

A number of different forms for a_d have been proposed. Legg and Raupach (1982) and Ley and Thompson (1983) argued heuristically that the term $\rho\partial\sigma_w^2/\partial z$ in the vertical component of the time-dependent Navier-Stokes equation is balanced by a mean-pressure-gradient which is accounted for in (3.14) by

$$a_d = \partial\sigma_w^2/\partial z. \tag{3.15}$$

Wilson *et al.* (1981b) applied a similar argument to the modified Langevin equation

$$d(W/\sigma_w) = -(W/\sigma_w t_L)dt + \left(\frac{2}{t_L}\right)^{1/2} d\mathcal{W}_t + (a'_d/\sigma_w)dt \tag{3.16}$$

to show

$$a'_d = \tfrac{1}{2}\,\partial\sigma_w^2/\partial z.$$

By expanding the term $d(W/\sigma_w)$, (3.16) can be recast in the form of (3.14) showing that the Wilson *et al.* correction is equivalent to

$$a_d = \tfrac{1}{2}(\partial\sigma_w^2/\partial z) + \tfrac{1}{2}(W^2/\sigma_w^2)\partial\sigma_w^2/\partial z. \tag{3.18}$$

The corrections (3.15) and (3.18) (and a third alternative proposed by Durbin (1983)) differ by terms in-

volving W^2/σ_w^2. In the limit of weakly inhomogeneous turbulence all three corrections are equivalent since then $\langle W^2 \rangle = \sigma_w^2$. However, for strongly inhomogeneous turbulence, Sawford's (1984b) calculations show $\langle W^2 \rangle \neq \sigma_w^2$ suggesting that these alternative corrections are not then equivalent.

An obvious constraint on the Langevin equation is that it should reproduce known Eulerian velocity statistics if the marked particles represent an unbiased sample of all particles in the flow. This is the case, for example, when the source is uniformly distributed or for the steady-state distribution of particles dispersing in a bounded region. Thompson (1984) rigorously derived the drift corrections (3.15) and (3.18) by matching the first few terms of appropriate moment expansions for such unbiased statistics. He showed that with increasing inhomogeneity, the standard form of the Langevin equation (3.14) with the drift correction (3.15) breaks down and that higher order moment corrections (involving $\partial\sigma_w^2/\partial z$) to the random velocity increment are necessary. This makes it impractical to model dispersion in strongly inhomogeneous turbulence using (3.14). On the other hand, Thompson's analysis of the modified Langevin equation (3.16) shows that the random velocity increment remains Gaussian and that the drift correction (3.18) works in arbitrarily strongly inhomogeneous turbulence. Durbin (1983) showed that this modified Langevin equation also correctly represents dispersion in nonstationary turbulence.

Comparisons of Langevin simulations with atmospheric dispersion data in the diabatic boundary layer have been reported by Wilson *et al.* (1981c) and Ley and Thompson (1983). The latter apply the Dyer-Hicks (Dyer, 1974) stability correction for heat transfer,

$$\phi_H = (1 + 5z/\mathcal{L}), \qquad \mathcal{L} > 0 \quad (3.19a)$$

$$= (1 - 16z/\mathcal{L})^{-1/2}, \quad \mathcal{L} < 0 \quad (3.19b)$$

where $\mathcal{L}$ is the Monin Obukov length, to the diffusivity in the usual way i.e.

$$K_H = ku_*z/\phi_H. \qquad (3.19c)$$

For stable conditions the height-dependence of σ_w was derived from the Minnesota data of Caughey *et al.* (1979), while in unstable conditions the formulation of Panofsky *et al.* (1977) was used:

$$\sigma_w/u_* = 1.5(1 - z/h_i), \qquad \mathcal{L} > 0 \quad (3.20a)$$

$$= 1.3(1 - 3z/\mathcal{L})^{1/3}, \quad \mathcal{L} < 0 \quad (3.20b)$$

where h_i is the height of the stable boundary layer.

The drift correction (3.15) was used and t_L was fixed by assuming asymptotic matching to the diffusion equation with the stability corrected forms of $K(z)$ and $\sigma_w(z)$. Allowing for step-size corrections near the surface, the simulations were in good agreement with concentration profiles from PPG and mean cloud-height from the Porton data.

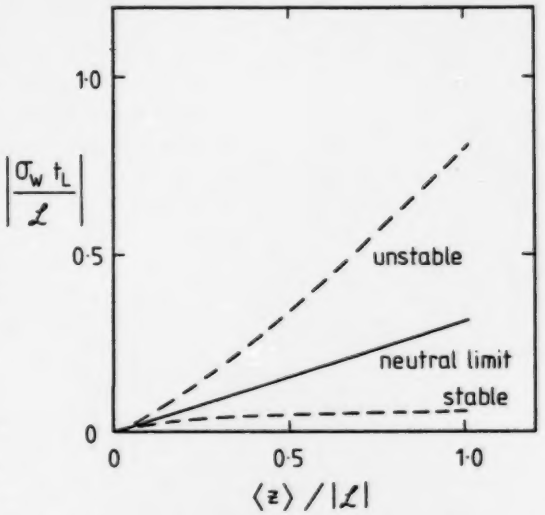

FIG. 2. Lagrangian length scale, $\sigma_w l_L = K_H/\sigma_w$, as a function of stability in the atmospheric boundary layer.

It is interesting to examine the effects of stability a little more closely. Figure 2 shows the length scale, $\sigma_w l_L$, calculated as K_H/σ_w from the diffusion matching procedure as a function of stability. (In the stable case the variation in σ_w/u_*, which is less than 10% under the conditions considered, has been ignored). By analogy with the neutral simulations reported by Sawford (1984b) and discussed earlier, the gradient of $\sigma_w l_L$ is a measure of the strength of the inhomogeneity in the turbulence. Clearly, increasing stability makes the turbulence less inhomogeneous and increasing instability increases the strength of the inhomogeneity. Physically the reason for this trend is that the influence of the boundary on the turbulence tends to be reduced in stable conditions and enhanced in unstable conditions. Thus the diffusion equation should be a better (worse) large-time approximation and concentration profiles should be more (less) nearly Gaussian with increasing (decreasing) stability. These conclusions are supported by the Langevin simulations of Ley and Thompson (1983) and by the data analysis and diffusion equation calculations of Nieuwstadt and van Ulden (1978). Figures 5 and 6 in Ley and Thompson show that the diffusion equation prediction for $\langle Z(t) \rangle$ is in excellent agreement with Langevin simulations[1] at $\langle Z \rangle/\mathcal{L} \sim 1$, slightly overestimates near neutral conditions (cf. Sawford's (1984b) neutral simulations) and overestimates increasingly with increasing $-\langle Z \rangle/\mathcal{L}$. Nieuwstadt and van Ulden (1978) show that the diffusion equation fits

[1] Ley and Thompson actually compare their Langevin simulations with the similarity theory of Chaudhry and Meroney (1973) who, however, determined the universal constants of the theory by matching to the diffusion equation predictions.

stable data very well but breaks down under unstable conditions. The profile shape factors they deduce from the data confirm the trend to Gaussianity with increasing stability.

d. Convective turbulence

Our detailed understanding of turbulence structure in the convective boundary layer (CBL) derives from field experiments (Kaimal *et al.*, 1976; Caughey and Palmer, 1979), laboratory experiments (Willis and Deardorff, 1974) and numerical experiments (Deardorff, 1974). These investigations show that the CBL can be idealized as a multilayer structure. Proceeding upwards from the surface we have:

(i) The surface layer ($z < |\mathcal{L}|$) where wind shear (and mechanical generation of turbulence) play a dominant role. We have already discussed application of the Langevin equation to this region in sections 3b and 3c.

(ii) The free convection layer ($|\mathcal{L}| < z < 0.1z_i$) where wind shear is no longer important, the turbulence is mainly generated by buoyancy forces and is strongly height dependent.

(iii) The mixed layer $0.1z_i < z < 0.8z_i$ where large buoyant motions dominate the turbulence which is thus independent of height but controlled by z_i.

(iv) The interfacial layer where the turbulence is strongly influenced by entrainment effects, the characteristics of the capping inversion and the stable atmosphere aloft.

Much of our understanding of dispersion from neutrally buoyant sources in the CBL derives from Lamb's (1978) [see also Lamb (1982)] simulations. Lamb modeled the Lagrangian vertical velocity by

$$W(t) = w_E[\underline{X}(t), t] + W_s, \qquad (3.21)$$

where $w_E(\underline{x}, t)$ is the Eulerian velocity field generated by Deardorff's (1974) large-eddy simulation of CBL turbulence and $\underline{X}(t)$ is the position of the particle at time t (similar equations were used for the other velocity components). In (3.21) W_s is a subgrid-scale velocity, modeled by the Langevin equation with $\sigma_w = q$ and $t_L = \Delta/q$ where $\Delta = 90$ m is the grid size and q^2 the subgrid-scale kinetic energy. Except near the surface and near the capping inversion, q is small and W is dominated by w_E, the resolved Eulerian field.

The most striking result of Lamb's simulations (since confirmed in the laboratory (Willis and Deardorff, 1978) and in the atmosphere (Moninger *et al.*, 1983) is that for elevated sources with $z_s > 0.1z_i$ the plume center line (the line of maximum mean concentration) descends and reaches the ground a dimensionless distance $\bar{x} \sim 2z_s/z_i$ downwind where the maximum mean dimensionless concentration, $\langle \bar{c} \rangle \sim 1.2z_i/z_s$, is observed. For $\bar{x} > 3$–4, contaminant is, on average, well-mixed throughout the CBL. Lamb pointed out that this centerline touch-down effect can be ascribed to the positive skewness in the distribution of the vertical velocity; contaminant is more likely to be emitted into sinking rather than rising air.

Much of the CBL is occupied by the mixed layer where turbulence length and time scales are large ($L \sim z_i$; $z_i/\sigma_w \sim 15$ min (Kaimal *et al.*, 1976)) and the turbulence is approximately homogeneous but with a positively skewed vertical velocity distribution. Weil and Furth (1981) idealized these features in a Lagrangian simulation in which it was assumed that the time scale is not just large, but infinite, that the mixed-layer occupies the whole of the CBL and that there is perfect reflection at the boundaries. Then the distribution of material throughout the CBL depends only on the skewed velocity distribution at the source. This model is a special case of the homogeneous Langevin equation (3.1) in which t_L is infinite and the initial velocity distribution is skewed.

Misra (1982) and Venkatram (1983) proposed analytical models based on similar simplifying assumptions. Crude models such as these capture (and indeed emphasize) the essential physics of dispersion from elevated sources in the CBL and show that mixed-layer turbulence plays a dominant role. Figure 2 of Weil (1983) shows that these models all perform well in the near-field and far-field but do less well for $\bar{x} \sim 2z_s/z_i$ where the maximum mean ground level concentration occurs. Clearly, at this intermediate range effects such as "loss of memory" of the initial velocity due to the finite timescale and the inhomogeneity of turbulence in the surface and free-convection layers cannot be ignored. A full Lagrangian (Langevin equation) simulation incorporating these effects (and the skewness of the vertical velocity distribution) has recently been carried out by Baerentsen and Berkowicz (1984) who report excellent agreement with the Willis and Deardorff (1976, 1978, 1981) laboratory experiments.

For neutrally buoyant ground-level sources (and for elevated sources after touchdown at $\bar{x} \sim 2z_s/z_i$) the laboratory experiments and Lamb's simulations show that the mean plume centerline rises away from the surface. Sawford (1984b) (see section 3b) showed that the Langevin model produces this "lift-off" phenomenon in strongly inhomogeneous turbulence and it is possible that the effect is observed in the CBL because of the large gradient in the length-scale $\sigma_w t_L$ in the free-convection region (see Fig. 2).

e. Buoyancy forces in stable stratification

We have already seen in section 3c that stable stratification tends to make boundary layer turbulence more nearly homogeneous. It also results in a restoring buoyancy force when a fluid particle is displaced from its equilibrium position. For moderate to strong stability, $NT > 1$, where N is the buoyancy frequency and T the Eulerian integral timescale of the turbulence, Csanady (1964) and Pearson *et al.* (1983) proposed generalized Langevin-type models for stratified ho-

mogeneous turbulence which include a buoyancy force. The particle equation of motion proposed by Pearson *et al.* is

$$\frac{dW}{dt} = -2\beta NW - g\rho'/\rho_0 + H(t), \qquad (3.22)$$

where β is a constant of O(1), ρ' is the density perturbation from the local mean value, ρ_0 the mean density and g the gravitational acceleration. Csanady's model leaves out the wave-damping term, $-2\beta NW$. Pearson *et al.* conclude that the results of the model are insensitive to the form of the random forcing function, $H(t)$.

Both Csanady and Pearson *et al.* supplement the equation of motion with an equation describing the exchange of material between marked particles and the ambient fluid by molecular diffusion,

$$\frac{d\rho'}{dt} = -\left(\frac{\partial\rho}{\partial z}\right)W - \gamma N\rho', \qquad (3.23)$$

where γ is a constant.

A number of limiting results were obtained analytically. Both models show that buoyancy forces inhibit vertical dispersion. For $\gamma = 0$ (no molecular mixing) vertical dispersion is finite,

$$\sigma_z^2 \sim \langle W^2\rangle/N^2 = \text{const}, \quad (t > N^{-1}). \qquad (3.24)$$

For finite but weak mixing, $\gamma \ll 1$, a reduced rate of growth occurs. Pearson *et al.* discuss experimental evidence for such reduced vertical dispersion.

4. Concentration fluctuations

a. Homogeneous turbulence without mean shear

We see from (2.2) that we need to consider two-particle displacement statistics in order to evaluate second order statistics of the concentration field. Thus, in addition to the "memory" effects modeled by the Langevin equation it is necessary to model the effect of the spatial structure of the turbulence on the relative motion of a pair of particles.

The mean-square concentration can be obtained from (2.2) by taking the limit $\underline{x}_1 \to \underline{x}_2$. Therefore, since we deal here with reversed diffusion, we are interested in the displacement statistics of a pair of particles in the limit of vanishing initial separation. Some of the subtleties of this limit are considered by Durbin (1980a), Sawford (1983a), and Sawford and Hunt (1985). Essentially, the outcome of these considerations is that for large Reynolds number and Peclet number molecular effects (diffusion, which is ultimately responsible for dissipation of concentration variance and viscosity) are accounted for implicitly if the limit $\underline{x}_1 \to \underline{x}_2$ is taken as an outer limit i.e., a limit on the scale L and explicit viscous and diffusive processes are ignored.

For analytic and numerical convenience all Lagrangian calculations of concentration fluctuations reported so far have been for instantaneous area sources for which (2.2), in the limit $\underline{x}_1 \to \underline{x}_2$, reduces in an obvious simplified notation, to the one-dimensional form

$$\langle c^2(z, t)\rangle = \iint_V P_2(z_1', z_2', 0; z, t)S(z_1')S(z_2')dz_1'dz_2'. \qquad (4.1)$$

In the context of atmospheric dispersion we are most interested in fluctuations arising from discrete sources. Little loss of generality is involved in choosing a Gaussian source distribution

$$S(z) = \frac{1}{(2\pi)^{1/2}\sigma_0}\exp\left(-\frac{z^2}{2\sigma_0^2}\right). \qquad (4.2)$$

The instantaneous plane source distribution (4.2) can be regarded as an approximation to a continuous line source provided the streamwise intensity of turbulence is small.

Various two-particle models have been proposed which involve a pair of coupled Langevin equations in which the rate of separation of the pair of particles is modulated according to their separation (Durbin, 1980a) or their expected separation (Lamb, 1981; Sawford, 1982) by a term involving the space structure function of the turbulence. The idea is to model the physical notion that particles tend to move together when their separation is small compared with L and to move inde-pendently when their separation is large compared with L.

With "separation" and "center of mass" variables, $\Delta = \frac{1}{\sqrt{2}}(Z_1 - Z_2)$ and $\Sigma = \frac{1}{\sqrt{2}}(Z_1 + Z_2)$ respectively, Durbin's (1980a) model equations are

$$\frac{d\Delta}{dt} = R^{1/2}(\Delta)W_1', \qquad (4.3a)$$

and

$$\frac{d\Sigma}{dt} = |2 - R(\Delta)|^{1/2}W_2', \qquad (4.3b)$$

where $R(\Delta)$ is an Eulerian structure function and W_1' and W_2' are independent Langevin velocities. A simple but appropriate form for $R(\Delta)$ is

$$R(\Delta) = [\Delta^2/(\Delta^2 + L^2)]^{1/3}. \qquad (4.4)$$

Equation (4.4) interpolates between the inertial range form, $R(\Delta) \sim (\Delta/L)^{2/3}$ for $\Delta \ll L$ (corresponding to the Eulerian velocity spectrum $(-5/3)$ inertial subrange) and the large scale limit $R(\Delta) \to 1$.

Pairs of molecular trajectories can be found by solving finite difference versions of (4.3) and (3.1). Details are given by Durbin (1980a). In addition to the constraint, $\delta t \ll t_L$, already referred to for mean field modeling, the step size must also satisfy the constraint $\delta t \ll (\Delta/L)R^{-1/2}(\Delta)t_L$ for $\Delta \geq \sigma_0$ in order to properly resolve the relative motion on scales of the source size

and larger. As noted by Sawford (1983a) concentration moments estimated by the backward dispersion process become increasingly uncertain with travel time (or distance) from the source, since as the particles disperse fewer pass through the source and hence fewer make non-zero contributions to concentration moment estimates. Nevertheless, typical one-dimensional (i.e. continuous line source or instantaneous area source) calculations using $N_t \sim 5 \times 10^4$ and 300 time steps per realization to reach $t/t_L = 10$ (which is well into the asymptotic stage of dispersion) are quite practicable. Calculations for higher dimensions are probably not.

An important property of (4.3) is that it is a nonlinear stochastic differential equation in which the rate of separation depends on the instantaneous separation. It yields a non-Gaussian distribution for Δ,

$$P(\Delta, t; \Delta_0, 0) = \frac{R^{-1/2}(\Delta)}{(2\pi)^{1/2}\sigma_z} \exp\left(-\frac{[G(\Delta) - G(\Delta_0)]^2}{2\sigma_z^2}\right), \quad (4.5)$$

where $G(\Delta) - G(\Delta_0) = \int_{\Delta_0}^{\Delta} R^{-1/2}(\Delta')d\Delta'$ and σ_z is the single particle dispersion (see section 3.1).

The essence of the models proposed by Lamb (1981) and Sawford (1982), in which the rate of separation depends on the expected separation, can be demonstrated by replacing $R(\Delta)$ by $\langle R(\Delta)\rangle$ in (4.3) to give for the rate of separation

$$\frac{d\Delta}{dt} = \langle R(\Delta)\rangle^{1/2} W_1'. \quad (4.6)$$

This is a linear equation and since W_1' is Gaussian (in homogeneous turbulence) so too are $d\Delta/dt$ and Δ. Sawford (1983a) showed that there are important qualitative differences in the magnitude of concentration fluctuations predicted by Durbin's nonlinear (and non-Gaussian) model and the linear models of Lamb (1981) and Sawford (1982) for which $P(\Delta)$ is Gaussian. This can be seen in Fig. 3 which shows the centerline squared intensity of fluctuations

$$s^2(0, t) = \frac{\langle c^2(0, t)\rangle}{\langle c(0, t)\rangle^2} - 1 \quad (4.7)$$

as a function of time. The important difference arises in the large-time limit where for Durbin's model, $s^2(0, t)$ asymptotes to a constant which is a function of the source size, σ_0,

$$s^2(0, t) \to 1.35\sigma_0^{-1/3} - 1 \quad (t \to \infty;\ \sigma_0 \ll L), \quad (4.8)$$

while for the linear models it is independent of source size and vanishes according to

$$s^2(0, t) \to \frac{1}{2}\rho^2 \sim t^{-1}, \quad (t \to \infty), \quad (4.9)$$

where $\rho = 1 - \langle\Delta^2\rangle/\sigma_z^2$ is the correlation between the positions of the two particles. For both models, for σ_0

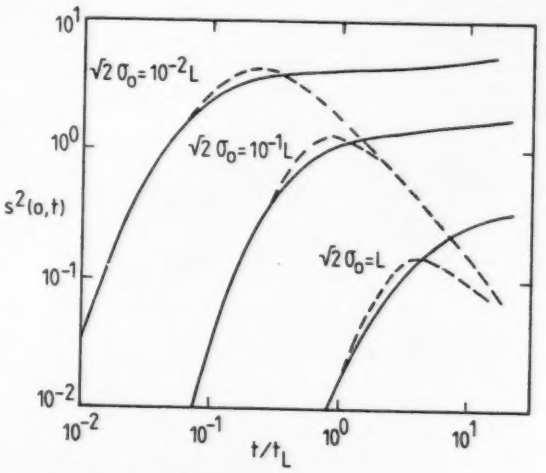

FIG. 3. Intensity of concentration fluctuations in stationary homogeneous turbulence. (Solid line), non-Gaussian particle separation pdf; (dotted line), Gaussian particle separation pdf.

$\ll L$ concentration fluctuations evolve on the time scale, $(\sigma_0/L)^{2/3}t_L$, a consequence of inertial range scaling.

By calculating separately the fluctuations due to meandering (i.e., bulk motion of the cloud of contaminant) and those due to the internal structure of the cloud (i.e., in coordinates relative to the center of mass) Sawford (1983a) explained the difference between (4.8) and (4.9) by showing that Gaussian models smooth out the internal structure of the cloud i.e., at large time the ensemble averaging in (4.6) is equivalent to spatial averaging over the cloud. Then concentration fluctuations are due entirely to meandering and consequently vanish. The nonlinearity of Durbin's model thus plays an essential role in accounting for the internal structure of the cloud and fluctuations in relative coordinates.

It is difficult to obtain direct evidence to conclusively support the asymptotic predictions of either Durbin's nonlinear model or the linear Gaussian models. Indirect support for Durbin's approach is provided by numerical simulations by Holloway and Kristmannsson (1984) of the dispersion of a tracer cloud in decaying geostrophic turbulence. These show, as does Durbin's model, that internal structure persists even when the tracer has been dispersed over distances substantially larger than the largest eddy length scales. Other evidence supporting Durbin's approach is discussed in section 4d. We note here that other theories of concentration fluctuations also give widely disparate predictions for the asymptotic value of s in stationary homogeneous turbulence. Chatwin and Sullivan's (1979) linear strain model predicts (for a three-dimensional cloud) that s^2 diverges like σ_z^n where n lies between 1 and 2. The Eulerian second-order-closure model of Sykes *et al.* (1984) predicts $s^2 \sim t^{-1/2}$ while Csanady's (1973) similarity model assumes s^2 to be constant along the centerline.

The spatial distribution of mean-square concentration is determined by the center of mass distribution and is Gaussian [exactly for the linear models and to an excellent approximation for Durbin's model (Sawford, 1983a)] with variance $\frac{1}{2}[\sigma_0^2 + (1 + \rho)\sigma_z^2]$. The square of the mean concentration is also Gaussian with variance $\frac{1}{2}(\sigma_0^2 + \sigma_z^2)$. These variances are generally different since $\rho > 0$, so in general $\langle c'^2(z, t)\rangle$ is not Gaussian. Near to the source, $\rho \to 1$ and $\langle c'^2(z, t)\rangle$ exhibits a double-peaked structure with the maximum fluctuations occurring off the center-line. Far from the source, $\rho \to 0$ and $\langle c'^2(z, t)\rangle$ approaches a Gaussian form. The transition from a double-peaked to a Gaussian distribution has been observed in wind tunnel measurements (Stapountzis *et al.*, 1985; Warhaft, 1984).

A second consequence of the different variances for $\langle c^2\rangle$ and $\langle c\rangle^2$ is that $\langle c'^2\rangle$ decays less rapidly with distance from the center line than does $\langle c\rangle^2$ so that the intensity of fluctuations increases rapidly with distance from the center line. This behavior has been widely observed (Murthy and Csanady, 1971; Stapountzis *et al.*, 1985; Fackrell and Robins, 1982; Sawford *et al.*, 1985).

b. *Sheared homogeneous turbulence*

Durbin (1980b) pointed out that the interaction of turbulent separation transverse to the mean wind with shear causes a pair of particles to separate in the direction of the mean wind. For a constant mean shear

$$\frac{d\bar{U}}{dz} = \gamma, \tag{4.10}$$

and ignoring streamwise turbulence,

$$\frac{d\Delta_x}{dt} = \gamma\Delta_z, \tag{4.11}$$

where $\Delta_x = 2^{-1/2}(X_1 - X_2)$. The vertical separation is now denoted by Δ_z and is given by (4.3a) but with the structure function evaluated at $\Delta = (\Delta_x^2 + \Delta_z^2)^{1/2}$ since the correlation between the particle velocities depends on the total separation.

It follows from (4.11) that Δ_x/Δ_z is $O(\gamma t)$. Thus shear is not important for times small compared with the shear time scale,

$$\Delta_x \ll \Delta_z, \quad (\gamma t \ll 1), \tag{4.12}$$

and concentration fluctuations are the same as for the unsheared case. For times large compared with the shear time scale, shear separation dominates the turbulent separation,

$$\Delta_x \gg \Delta_z, \quad (\gamma t \gg 1) \tag{4.13}$$

and the vertical separation equation (4.3a) reduces to

$$\frac{d\Delta_z}{dt} \cong R(\Delta_x)W'_1, \tag{4.14}$$

which is a linear equation and so results in a Gaussian distribution for Δ_z. Thus concentration fluctuations are smoothed out and the intensity of fluctuations vanishes like (4.9).

Figure 4 shows model predictions for $s^2(0, t)$ for a range of source sizes and shear strength. Two timescales are relevant. These are the time for development of fluctuations in unsheared homogeneous turbulence, $(\sigma_0/L)^{2/3}t_L$, and the shear time scale, γ^{-1}. For $(\sigma_0/L)^{2/3}\gamma t_L \ll 1$ (i.e., for sufficiently small sources or weak shear) the asymptotic level (4.8) is reached before shear begins to reduce fluctuations. Conversely for $(\sigma_0/L)^{2/3}\gamma t_L \gg 1$, the fluctuations begin to decay before the limit (4.8) is reached.

The only measurements with which these predictions can be compared are those of Tavoularis and Corrsin (1981) for the temperature fluctuations downstream of a continuously heated rod in sheared homogeneous turbulence in a wind tunnel. Figure 5 shows the squared intensity of fluctuations calculated from their Fig. 2 and plotted as a function of distance from the source (in units of the tunnel height). As a rough guide for comparison with the theory (which is for an instantaneous source) note that for these continuous-source experiments $\gamma^{-1} \cong 0.025$, the center line mean wind speed, $\bar{U}_c \cong 12$ m s^{-1} and $h = 30$ cm so that $\gamma t = 1$ corresponds to $x/h \cong 0.8$, i.e., Fig. 5 corresponds to $\gamma t \gg 1$ and so represents the shear-dominated regime. The near-linear fall-off in $s^2(0, x)$ thus supports the theoretical prediction (4.9).

c. *Neutral boundary layer*

We restrict attention to the constant stress region where the length scale is proportional to distance from

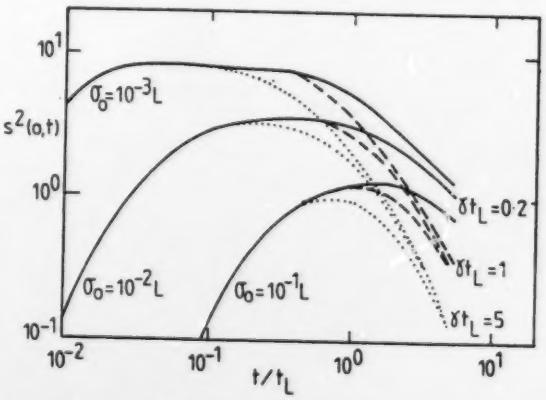

FIG. 4. Effect of mean shear on the intensity of concentration fluctuations in homogeneous turbulence according to Durbin's (1980a) model.

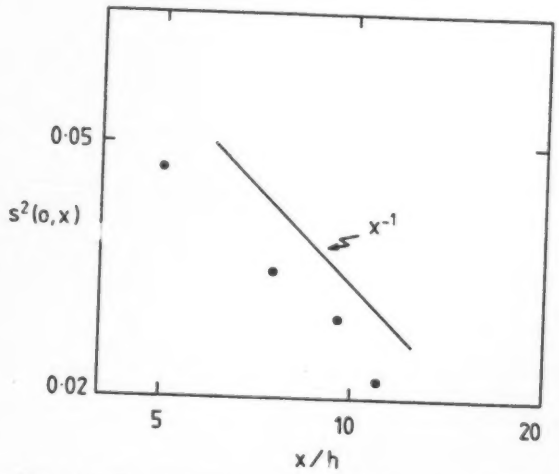

FIG. 5. Intensity of temperature fluctuations downstream of a continuously heated rod in sheared homogeneous turbulence in a wind tunnel (data from Tavoularis and Corrsin, 1981).

the boundary, $\sigma_w t_L \cong 0.3z$ (see section 3b) and σ_w is constant and given by (3.9). Sawford (1983b) modeled the effect of the increasing scale of turbulence simply by using local values of t_L and L in the model equations for homogeneous turbulence. In the two-particle case these were evaluated at the center of mass of the pair of particles, $Z_m = \sqrt{1/2}\Sigma = 1/2(Z_1 + Z_2)$. With the usual logarithmic mean wind profile, (4.11) becomes

$$\frac{d\Delta_x}{dt} = \frac{u_*}{k\sqrt{2}} \ln(Z_1/Z_2). \tag{4.15}$$

As with the single particle case, the time scale z_s/u_* represents the time for which the source height influences dispersion. For $t \gg z_s/u_*$, all memory of the release height is lost and dispersion proceeds as for a ground-level release. In this stage the cloud grows linearly with height and as shown by Hunt and Weber (1979), $\langle \Delta_z^2 \rangle$ (effectively the mean-square instantaneous vertical dimension of the cloud) remains a constant fraction of the single-particle dispersion, $\langle Z_1^2 \rangle - \langle Z_1 \rangle^2$ (effectively the mean-square width of the envelope of the cloud). In physical terms, as the cloud grows the meandering motions of the center of mass persist because increasingly large eddies are encountered as it rises through the boundary layer. Sawford's calculations give $\langle \Delta_z^2 \rangle / (\langle Z_1^2 \rangle - \langle Z_1 \rangle^2) = 0.72$, in good agreement with the rough theoretical estimate of 0.64 obtained by Hunt and Weber (1979) for the same σ_w and t_L. Figure 6 shows the effect of the inhomogeneity and of mean shear on the intensity of fluctuations for a top-hat source distribution. We see again that at small time, $t \ll z_s/u_*$, the inhomogeneity and shear are unimportant and for small enough sources, $[d_0/L(z_s)]^{2/3} t_L(z_s) < z_s/u_*$, the homogeneous asymptotic limit (4.8) [in fact the equivalent result for the top-hat source (Durbin, 1980a)] is reached before the influence of shear and inhomogeneity is felt.

For $t \gg z_s/u_*$, shear and inhomogeneity have important effects. The inhomogeneity alone causes the intensity of fluctuations to increase with time as the ever increasing scale of turbulence and the persisting center of mass motions take effect. As with the homogeneous case, shear smooths and reduces concentration fluctuations but now competes against the tendency of the inhomogeneity to increase the intensity of fluctuations. The net result of these opposing influences is that for $t \gg z_s/u_*$, $s^2(z_s, t)$ is constant and (contrary to the homogeneous case) independent of source size.

These results agree well with the wind tunnel measurements of Fackrell and Robins (1982) and Raupach and Legg (1983). Figure 6 reproduces all the qualitative features in both Fig. 5 of Fackrell and Robins and Fig. 5 of Raupach and Legg. Indeed there is remarkable similarity between the model and experiment. Quantitatively the asymptotic limit from Fig. 6, $s^2(z_s, t) \sim 0.2$, agrees quite well with Raupach and Legg's measured value of $\sim$0.25 for a line source. For a "point" source the measurements of Fackrell and Robins give a higher value of $\sim$0.3–0.4 as is expected.

d. *Multiple sources*

While the mean concentration can be obtained by adding contributions of individual sources, fluctuations in general are not additive because of the imperfect correlation between the concentration contributions from separate sources. For a pair of sources (denoted by subscripts 1, 2) this correlation is defined in the usual way by

$$\rho_c = \langle c_1' c_2' \rangle / \langle c_1'^2 \rangle^{1/2} \langle c_2'^2 \rangle^{1/2}. \tag{4.16}$$

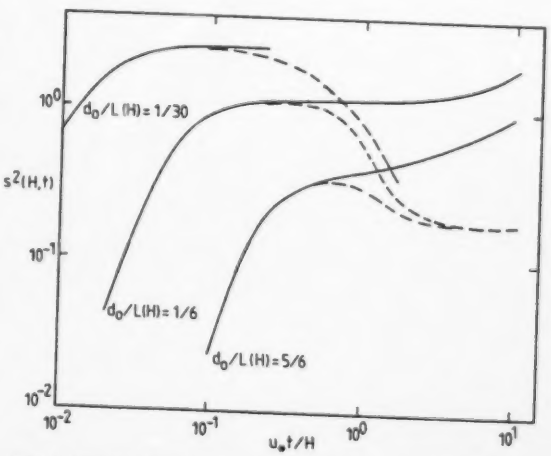

FIG. 6. Intensity of concentration fluctuations in a neutral boundary layer according to Sawford's (1983b) extension of Durbin's (1980a) model.

We have calculated ρ_c for a pair of instantaneous plane Gaussian sources (see (4.2)) separated by a distance d in stationary homogeneous turbulence. As for a single source, the nonlinearity in Durbin's (1980a) equation for the rate of separation of particle pairs has a profound influence. Figure 7 shows the correlation on the center line between the two sources, $\rho_c(0, t)$, as a function of travel time for a range of source separations within the inertial subrange. Near to the source the correlation becomes increasingly negative as the two separated plumes tend to meander synchronously so that at any instant one or the other is sampled on the center line but not both. With increasing travel time the plumes begin to overlap, meandering becomes less important and the correlation passes through a minimum and then increases. Perhaps the most striking result is that at large time, $t \gg (d/L)^{2/3} t_L$, ρ_c asymptotes to a constant value, which is not unity and is a function of the source separation. In fact,

$$\rho_c \to \frac{(d/\sqrt{2}L)^{-1/3} - 1}{[2^{1/3}\Gamma(1/3)/(2\pi)^{1/2}](L/\sigma_0)^{1/3} - 1}, \quad t \to \infty \quad (\sigma_0, d) \ll L. \tag{4.17}$$

Thus, Durbin's (1980a) nonlinear model predicts that in stationary homogeneous turbulence, two separated plumes never fully mix and the extent of the unmixedness depends on their initial separation. This behavior is analogous to the source-size dependence and patchiness or internal structure discussed by Sawford (1983a) for single sources (see Section 4a).

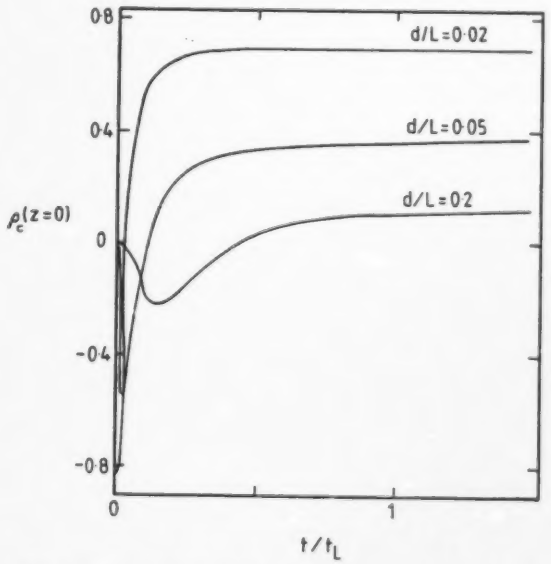

FIG. 7. Correlation between the concentration contributions from two separated sources in homogeneous turbulence (calculated on the centreline between the sources) as a function of time for indicated separations according to Durbin's (1980a) model.

For linear or Gaussian models (Sawford, 1982; Lamb, 1981)

$$\rho_c \to 1, \quad t \to \infty, \tag{4.18}$$

thus indicating complete mixing and no source-separation dependence.

Warhaft's (1984) temperature fluctuation measurements downstream of a separated pair of heated wires in grid turbulence in a wind tunnel (see his Figs. 14–17) show an asymptotic value for $\rho_c(0, t = x/\bar{U})$ which differs from unity and is a function of the wire separation. They thus provide qualitative support for the predictions of Durbin's model. In the atmosphere, boundary layer measurements for a pair of ground-level sources separated in the crosswind direction also indicate (albeit with rather more scatter) that ρ_c does not asymptote to unity (Sawford *et al.*, 1985).

Durbin (1982) has also used his model to calculate the decay of temperature fluctuations downstream of a set of equally spaced parallel line sources in grid turbulence (the Warhaft and Lumley (1978) mandoline experiment). The important feature of these experiments that is reproduced by the model is that the rate of decay of the temperature fluctuations depends on the length scale of the initial temperature fluctuation field i.e., on the spacing of the source wires.

5. Conclusions

We have attempted to review recent work on Lagrangian statistical modeling of turbulent dispersion using the Langevin or Markov-chain approach in a critical and systematic way. Thus we first introduced the Langevin equation as a model for independent particle trajectories, and hence the mean concentration field, in stationary homogeneous turbulence. Even in this simple case a rigorous derivation is lacking and the Langevin model must be justified heuristically by the parallel between its properties and known properties of the turbulence.

Extensions to more complicated types of turbulence were then introduced successively. For the constant stress region of a neutral boundary layer, where the velocity scale is constant but length and time scales increase linearly with distance from the surface, it was assumed that the particle motion adjusts to the local value of the time scale. The choice of values for constants entering the specification of the turbulence scales was justified by matching the Langevin solution to the small-time homogeneous turbulence limit for an elevated source (an exact result) and to the large-time diffusion limit (a good approximation for the weakly inhomogeneous turbulence in a neutral boundary layer). Prediction of the Langevin equation are in good agreement with wind tunnel measurements but some inconsistencies show up in reported comparisons with atmospheric dispersion data.

When the turbulence velocity scale, σ_w, varies spatially, for example in crop-canopies or non-neutral boundary layers, an unphysical accumulation of par-

ticles results if it is merely assumed that the particle motion adjusts to the local value of σ_w. In this case a drift correction is necessary to account for the drift of particles up the gradient in σ_w^2. Again the form of this correction was justified by appealing to a special case, namely by requiring that a uniform concentration field be maintained.

In addition to its effect through the gradient in σ_w, thermal stability also influences the strength of the inhomogeneity of boundary layer turbulence. By suppressing vertical motion, an increase in stability reduces the influence of the boundary and makes the turbulence more nearly homogeneous, with the result that the diffusion equation is a better large-time approximation and concentration profiles are more nearly Gaussian than under neutral conditions. Increasing instability has the opposite effect resulting, in particular, in the failure of the diffusion equation. This is reflected both in laboratory convection tank experiments and Langevin simulations of strongly inhomogeneous turbulence by the "lift-off" of the maximum concentration from the surface and a counter-gradient flux below the maximum.

In convectively mixed layers skewness in the vertical velocity distribution plays an important role in the dispersion from neutrally buoyant sources. Langevin simulations with a finite time scale have been reported for this case but even simple models assuming an infinite timescale reproduce many of the observed features.

Application of Langevin simulations to the prediction of concentration fluctuations is less advanced. The significant extension from mean-field applications is the need to model particle-pair statistics and in particular the interdependence of the motion of pairs of particles. This has been achieved through the use of a pair of coupled Langevin equations, but the large-time asymptotic behavior of predicted concentration fluctuations in homogeneous turbulence depends crucially on whether the rate of separation of the pair of particles depends directly on the instantaneous separation, giving a nonlinear stochastic differential equation for the separation, or on the mean-square separation, giving a linear equation. In the former case, for a discrete source, the intensity of fluctuations is asymptotically constant and a function of source size. In the latter case because of smoothing of the internal structure of the plume, the asymptotic intensity of fluctuations vanishes and is independent of source size.

For other source configurations similar fundamental differences show up. The common element of the predictions of the nonlinear separation equation is that the asymptotic behavior of concentration fluctuations is dependent on the source length scale and represents a state of incomplete mixing. This result is receiving increasing support from wind tunnel experiments.

The nonlinear model has been extended to include the effect of a mean wind shear by accounting for the shear-induced streamwise separation of particle pairs. The main conclusion, in qualitative agreement with wind tunnel experiments, is that for times large compared with the shear time scale, concentration fluctuations are smoothed and the intensity of fluctuations decays linearly with time.

Extension to a neutral boundary layer using the "local turbulence" assumption has also been carried out. An important difference from homogeneous turbulence is that as a cloud grows meandering motions persist because increasingly large eddies are encountered as it extends through the boundary layer. The model predicts a constant asymptotic intensity of fluctuations which, unlike the homogeneous case, is not a function of source size and results from a balance between the competing effects of mean shear and the turbulence inhomogeneity.

APPENDIX

Nomenclature

a_d	drift correction; see Eq. (3.14)
c	concentration
$\tilde{c}$	nondimensional concentration; $\tilde{c} = cz_i^2\bar{U}/Q$
d	source separation
d_0	top-hat source half-width
$d\mathcal{W}_t$	Gaussian white-noise stochastic process
g	gravitational acceleration
h	wind tunnel height; see Fig. 5
h_s	stable boundary layer height
$H(t)$	random forcing function; see Eq. (3.19)
k	von Karman constant
K	turbulent diffusivity
L	Eulerian integral length scale
$\mathcal{L}$	Monin Obukov length
N_t	number of realizations
N	buoyancy frequency
$P(\Delta, t; \Delta_0, 0)$	particle separation pdf
$P_1(\underline{x}', t'; \underline{x}, t)$	single particle displacement pdf
$P_2(\underline{x}_1', x_2', t'; \underline{x}_1, x_2, t)$	two-particle displacement pdf
q^2	sub-grid-scale turbulence kinetic energy
Q	source strength
$R(\Delta)$	Eulerian structure function
Re	turbulence Reynolds number
$R_L(t)$	Lagrangian velocity autocorrelation
s	concentration fluctuation intensity
S	source distribution
t, t'	time
t_L	Lagrangian integral time scale
t_k	Kolmogorov time scale
T	Eulerian integral time scale
u_*	friction velocity
$\bar{U}$	mean wind speed

w_*	convective velocity scale
$W(t)$	Lagrangian vertical velocity
W_s	sub-grid-scale Lagrangian velocity
$\underline{x} = (x, y, z)$	Eulerian coordinate
$\tilde{z}$	nondimensional distance; $\tilde{x} = xw_*/\bar{U}z_i$
$\underline{X}$	Lagrangian coordinate
z_i	height of CBL capping inversion
z_s	source height
Z	Lagrangian vertical coordinate
Z_m	center of mass of particle pair; $\frac{1}{2}(Z_1 + Z_2)$
δt	time step
Δ	particle "separation"; $\Delta = (Z_1 - Z_2)/\sqrt{2}$
ρ	correlation between positions of a pair of particles
ρ_c	concentration correlation for a pair of sources; see Eq. (4.15)
ρ_0	mean density
ρ'	density perturbation
σ_0	source size, see Eq. (4.2)
σ_z	single particle dispersion
σ_Δ	rms particle separation
σ_w	Langevin velocity scale
σ_{wE}^2	Eulerian vertical velocity variance
Σ	particle "center of mass"; $(Z_1 + Z_2)/\sqrt{2}$
ϕ_H	Dyer-Hicks stability correction for heat transfer
$\langle\ \rangle$	ensemble average

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